Wim Buijs

List of Publications by Year in descending order

19 papers	293 citations	840776 11 h-index	888059 17 g-index
19 all docs	19 docs citations	19 times ranked	448 citing authors

#	Article	IF	Citations
1	Molecular Modeling Study to the Relation between Structure of LPEI, Including Water-Induced Phase Transitions and CO₂ Capturing Reactions. Industrial & Engineering Chemistry Research, 2021, 60, 11309-11316.	3.7	8
2	Molecular Modeling Study of the SO₂ Deactivation of an Amine Resin and a Procedure To Avoid SO₂ Deactivation Using a Polyethylene Glycol/Tertiary Amine System. Industrial & Engineering Chemistry Research, 2020, 59, 13388-13395.	3.7	3
3	Direct Air Capture of CO₂ with an Amine Resin: A Molecular Modeling Study of the Deactivation Mechanism by CO₂. Industrial & Engineering Chemistry Research, 2019, 58, 14705-14708.	3.7	10
4	Direct Air Capture of CO₂ with an Amine Resin: A Molecular Modeling Study of the Oxidative Deactivation Mechanism with O₂. Industrial & Engineering Chemistry Research, 2019, 58, 17760-17767.	3.7	13
5	Molecular structure of dextran sulphate sodium in aqueous environment. Journal of Molecular Structure, 2018, 1156, 320-329.	3.6	14
6	CO2 solubility in small carboxylic acids: Monte Carlo simulations and PC-SAFT modeling. Fluid Phase Equilibria, 2018, 458, 1-8.	2.5	7
7	Molecular Modeling Study toward Development of H₂S-Free Removal of Iron Sulfide Scale from Oil and Gas Wells. Industrial & Engineering Chemistry Research, 2018, 57, 10095-10104.	3.7	24
8	Direct Air Capture of CO₂ with an Amine Resin: A Molecular Modeling Study of the CO₂ Capturing Process. Industrial & Engineering Chemistry Research, 2017, 56, 12297-12304.	3.7	27
9	Thermodynamic and Transport Properties of Crown-Ethers: Force Field Development and Molecular Simulations. Journal of Physical Chemistry B, 2017, 121, 8367-8376.	2.6	15
10	Solubility of sulfur compounds in commercial physical solvents and an ionic liquid from Monte Carlo simulations. Fluid Phase Equilibria, 2017, 433, 50-55.	2.5	29
11	Atomistic understanding of cation exchange in PbS nanocrystals using simulations with pseudoligands. Nature Communications, 2016, 7, 11503.	12.8	48
12	Crystal structure, stability, and electronic properties of hydrated metal sulfates MSO4(H2O)n (M=Ni,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 77-86.	3.8	13
13	Correlation between Quantumchemically Calculated LUMO Energies and the Electrochemical Window of Ionic Liquids with Reduction-Resistant Anions. International Journal of Electrochemistry, 2012, 2012, 1-6.	2.4	27
14	Shape-selective synthesis of 2,6-diisopropylnaphthalene on H-mordenite catalysts. Journal of Catalysis, 2012, 292, 181-187.	6.2	10
15	Reply to the â€œComments on Shape-selective diisopropylation of naphthalene in H-mordenite: Myth or reality?â€• by Gyula Tasi and IstvÃ¡n PÃ¡linkÃ³. Journal of Catalysis, 2011, 279, 231.	6.2	1
16	Reply to the letter of Robert Brzozowski concerning the conclusions drawn in â€œShape-selective diisopropylation of naphthalene in H-Mordenite: Myth or reality?â€• Journal of Catalysis, 2011, 280, 142-143.	6.2	2
17	Catalytic and molecular separation properties of Zeogrids and Zeotiles. Catalysis Today, 2011, 168, 17-27.	4.4	15
18	Shape-selective diisopropylation of naphthalene in H-Mordenite: Myth or reality?. Journal of Catalysis, 2010, 270, 60-66.	6.2	16

#	Article	IF	Citations
19	Separation of diisopropylnaphthalene isomers. Journal of Chromatography A, 2009, 1216, 6410-6416.	3.7	11